

T_c and Δ_o in a Phenomenological “Pseudogap” Model

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We study numerically superconductivity in a system characterized by the presence of a phenomenological “pseudogap”, E_g , in the energy spectrum, for $0 \leq T \leq T^*$. T^* is a crossover temperature. As a simplification, the pseudogap and the superconducting gap have the same s -wave symmetry. We find that for $\forall E_g \neq 0$ we require a critical value of the superconducting interaction, V_d , to produce a finite superconducting critical temperature, T_c and another one for $\Delta_o \neq 0$.

1 Introduction

After their discovery by Bednorz and Muller[1] in 1986, the high-temperature superconductors (*HTSC*) are still attracting a lot of interest due to their unusual physical properties, both in the normal and in the superconducting phases. For example, the *HTSC* exhibit a pseudogap in the energy spectrum in the temperature range $0 \leq T \leq T^*$. T^* is defined by Maier et al.[2] as the crossover temperature where the spin-susceptibility is a maximum.

There is experimental evidence by the group of Tallon and Loram[3] where the pseudogap persists below T_c , being independent of the superconducting gap. This interpretation is in agreement with the experiment of energy gap evolution in the tunneling spectra of *Bi2Sr2CaCu2 δ* performed by Dipasupil et al.[4]. They find that the pseudogap smoothly develops into the superconducting state gap with no tendency to close at T_c . Another proof that the pseudogap and the superconducting gap are independent of each other is given in the experiments of Krasnov et al.[5] where they apply a magnetic field to their superconducting samples and they destroy the superconducting gap, but the pseudogap remains. They conclude that the pseudogap and the superconducting gap coexist in *Bi-2212* using intrinsic tunneling spectroscopy.

Rubio Temprano, Trounov and Müller[6] have recently studied the isotope effects on the pseudogap in the high-temperature superconductor *La_{1.81}Ho_{0.04}Sr_{0.15}CuO₄* by neutron crystal field spectroscopy. They have found evidence for the opening of an electronic pseudogap at $T^* \approx 60K$, above the superconducting critical temperature, $T_c \approx 32K$.

We exploit the consequences of the pseudogap on two macroscopic quantities in the superconducting state, namely, the superconducting critical temperature, T_c , and the superconducting order parameter at $T = 0$, Δ_o .

This paper is organized as follows. In Section 2, we

present the pseudogap model, following the steps of Tifrea, Grosu and Crisan[7]. In Section 3 we present our numerical results. In Section 4 we present our discussion and conclusions.

2 The “pseudogap” model

We assume[7] that the *PG* and the normal one-particle self-energy are given by

$$\Sigma(\vec{k}, i\omega_n) \equiv -E_g^2 G_o(\vec{k}, -i\omega_n) \quad , \quad (1)$$

where $G_o(\vec{k}, i\omega_n)$ is the free one-particle Green function. \vec{k} is the wave vector and $\omega_n = 2\pi T(n + 1/2)$ is the odd Matsubara frequency, with n an integer. With this choice of self-energy (Eq. (1)) is easy to show that the “*PG*” Green function is given by

$$G(\vec{k}, i\omega_n) = \frac{u_{\vec{k}}^2}{i\omega_n - E_{\vec{k}}} + \frac{v_{\vec{k}}^2}{i\omega_n + E_{\vec{k}}} \quad , \quad (2)$$

where we have chosen the pseudogap of pure s -symmetry, since we want to look for details overlooked in Ref. [7]. For example, the authors of Ref. [7] did not find critical pairing interactions to have $T_c \neq 0$ and $\Delta_o \neq 0$. These considerations have been properly taken into account by Pistolesi and Nozières[8] in a similar model to ours. A word of caution is in order here. The model we are discussing here appears to be more of a semiconductor type, as recognized in Ref. [8]. To transform the present model into a real pseudogap model, we should include a damping factor, as it has been done by Andrenacci and Beck[9].

The superconducting state in the *HTSC* is obtained from the two two *BCS* equations as follows

$$\begin{aligned} G^{-1}(\vec{k}, i\omega_n)\mathcal{G}(\vec{k}, i\omega_n) + \Delta\mathcal{F}^\dagger(\vec{k}, i\omega_n) &= 1 \\ \Delta^*\mathcal{G}(\vec{k}, i\omega_n) - G^{-1}(\vec{k}, -i\omega_n)\mathcal{F}^\dagger(\vec{k}, i\omega_n) &= 0 \end{aligned} \quad (3)$$

where $\mathcal{G}(\vec{k}, i\omega_n)$ and $\mathcal{F}^\dagger(\vec{k}, i\omega_n)$ are the diagonal and off-diagonal *BCS* Green functions, respectively. This interpretation of the *PG* is equivalent to make the following choice in the *T*-matrix approximation[10, 11, 12] for the superconducting self-energy:

$$\Sigma(\vec{k}, i\omega_n) = \begin{pmatrix} \Sigma(\vec{k}, i\omega_n) & \Delta \\ \Delta^* & \Sigma(\vec{k}, i\omega_n) \end{pmatrix} \quad (4)$$

This assumption produces two gaps, one coming from the *PG* and the other one from Δ in Eq. (4). Our approach is completely different from the one in Refs. [13-16] where they have an effective gap, given by $\Delta_{eff} = \sqrt{\Delta^2 + E_g^2}$. Their approach is equivalent to taking $\Delta = 0$ in our Eq. (4) and substituting $\Sigma(\vec{k}, i\omega_n)$ by the diagonal self-energy (Eq. (1)), with $E_g \rightarrow \sqrt{E_g^2 + \Delta^2}$.

Solving Eq. (3), we obtain

$$\mathcal{G}(\vec{k}, i\omega_n) = \sum_{i=1}^4 \frac{\alpha_i(\vec{k})}{i\omega_n - \omega_i(\vec{k})} ; \quad (5)$$

$$\mathcal{F}(\vec{k}, i\omega_n) = \Delta \sum_{i=1}^4 \frac{\beta_i(\vec{k})}{i\omega_n - \omega_i(\vec{k})} , \quad (6)$$

where

$$\omega_{\pm}^2 = E_k^2 + \frac{|\Delta|^2}{2} \pm |\Delta| \sqrt{E_g^2 + \frac{|\Delta|^2}{4}} \quad (7)$$

$$\omega_1(\vec{k}) = |\omega_+| ; \quad \omega_2(\vec{k}) = -|\omega_+| ; \quad \omega_3(\vec{k}) = |\omega_-| \quad (8)$$

$$\omega_4(\vec{k}) = -|\omega_-| ; \quad E_k^2 \equiv \epsilon^2(\vec{k}) + E_g^2 , \quad (9)$$

and $\epsilon(\vec{k}) = -2t(\cos(k_x) + \cos(k_y))$ is the free tight binding band in two dimensions. We are not considering here the presence of the chemical potential, which we leave for a future publication [17]. In Section 3 we choose $t = 1$, as our unit of energy. In Eqs. (5–6), the spectral weights, $\alpha_i(\vec{k})$ (normal ones) and $\beta_i(\vec{k})$ (superconducting ones), with $i = 1, 2, 3, 4$, are given by

$$\begin{aligned} \alpha_1(\vec{k}) &= \frac{\left(\frac{u_k^2}{\omega_1(\vec{k})+E_k} + \frac{v_k^2}{\omega_1(\vec{k})-E_k}\right)^{-1} \left((\omega_1)^2 - (\epsilon(\vec{k}))^2\right)}{4\Delta \omega_1(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \\ \alpha_2(\vec{k}) &= \frac{\left(\frac{u_k^2}{\omega_1(\vec{k})-E_k} + \frac{v_k^2}{\omega_1(\vec{k})+E_k}\right)^{-1} \left((\omega_1)^2 - (\epsilon(\vec{k}))^2\right)}{4\Delta \omega_1(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \\ \alpha_3(\vec{k}) &= \frac{-\left(\frac{u_k^2}{\omega_3(\vec{k})+E_k} + \frac{v_k^2}{\omega_3(\vec{k})-E_k}\right)^{-1} \left((\omega_3)^2 - (\epsilon(\vec{k}))^2\right)}{4\Delta \omega_3(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \\ \alpha_4(\vec{k}) &= \frac{-\left(\frac{u_k^2}{\omega_3(\vec{k})-E_k} + \frac{v_k^2}{\omega_3(\vec{k})+E_k}\right)^{-1} \left((\omega_3)^2 - (\epsilon(\vec{k}))^2\right)}{4\Delta \omega_3(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \\ \beta_1(\vec{k}) &= -\beta_2(\vec{k}) = \frac{(\omega_1)^2 - (\epsilon(\vec{k}))^2}{4\Delta \omega_1(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \\ \beta_3(\vec{k}) &= -\beta_4(\vec{k}) = \frac{(\omega_3)^2 - (\epsilon(\vec{k}))^2}{4\Delta \omega_3(\vec{k}) \sqrt{E_g^2 + \frac{|\Delta|^2}{4}}} \end{aligned} \quad (10)$$

We have to solve the T_c equation and the gap equation, Δ_o , at $T \equiv 0$. They are given by

$$\begin{aligned} \frac{1}{V_d} &= \frac{1}{N_x \times N_y} \sum_{n_x, n_y} \frac{1}{2\sqrt{(\epsilon(\vec{k}))^2 + E_g^2}} \\ &\times \tanh\left(\frac{\sqrt{(\epsilon(\vec{k}))^2 + E_g^2}}{2k_B T_c}\right) \equiv F(T_c) \end{aligned} \quad (11)$$

$$\frac{1}{V_d} = \frac{1}{N_x \times N_y} \sum_{n_x, n_y} \frac{1}{2\Delta_o \sqrt{\Delta_o^2 + 4E_g^2}} \times \left(\frac{A_o^2}{\sqrt{(\epsilon(\vec{k}))^2 + A_o^2}} - \frac{B_o^2}{\sqrt{(\epsilon(\vec{k}))^2 + B_o^2}} \right) \quad (12)$$

$$\begin{aligned} A_o^2(B_o^2) &\equiv E_g^2 + \frac{1}{2} \left(\Delta_o^2 \pm \Delta_o \sqrt{\Delta_o^2 + 4E_g^2} \right) \\ &= E_g^2 + \frac{1}{2} \left(\Delta_o^2 \pm \Delta_{eff}^2 \right) \end{aligned} \quad (13)$$

where $k_x = 2n_x\pi/N_x$ and $k_y = 2n_y\pi/N_y$, with $n_x = 0, 1, \dots, N_x - 1$, and $n_y = 0, 1, \dots, N_y - 1$, since we are solving our discrete system in two dimensions. We have chosen $N_x = N_y = 1000$ in our numerical calculations. V_d is the absolute value of the pairing interaction. We have used a precision of 10^{-5} to solve Eqs. (11-12). From these equations we conclude that $A_o^2 = \Delta_o^2$ and $B_o^2 = 0$ when $E_g = 0$.

3 Numerical results

In Fig. 1 we present T_c vs V_d for several values of the pseudogap parameter, E_g , for the case of pure s -wave symmetry. We observe that there is a critical value of the interaction potential, $V_{d,c}^{T_c}$, in order to have T_c . As we will see in the results for Δ_o vs V_d , there is also a critical value of the pairing potential below which $\Delta_o = 0$. In the case of $V_{d,c}$ coming from the $\Delta_o \rightarrow 0$, these two critical pairing interactions are different. These critical pairing interactions were not discussed in Ref. [7]. However, they were considered in a similar model by Pistoiesi and Nozières[8].

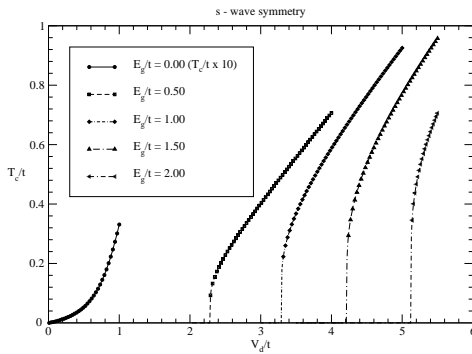


Figure 1. T_c/t vs V_d/t for several values of the pseudogap parameter, E_g/t , for the case of pure s -wave symmetry. For $E_g/t \neq 0$ there is a critical interaction potential, $V_d/t = V_{d,c}^{T_c}/t$, below which $T_c/t = 0$. For example, for $E_g/t = 0.50$ we find $V_{d,c}^{T_c}/t \approx 2.25$ in units of t .

In Fig. 2 we present Δ_o vs V_d for several values of E_g , when the pseudogap and the superconducting order parameter, at $T = 0$, have the same symmetry, namely, pure s -wave. We need a critical interaction potential, $V_{d,c}^{\Delta_o} \neq 0$,

when $E_g \neq 0$, in order to have $\Delta_o \neq 0$. From Fig. 2, for $E_g = 0.50$, $V_{d,c}^{\Delta_o} \approx 3.00$. Comparing Figs. 1 and 2, we see that for a fixed value of E_g , $V_{d,c}^{T_c} \leq V_{d,c}^{\Delta_o}$. This result implies that the ratio $2\Delta_o(V, E_g)/k_B T_c(V, E_g)$ is well defined only for $V \geq V_{d,c}^{\Delta_o}$, for a fixed value of E_g .

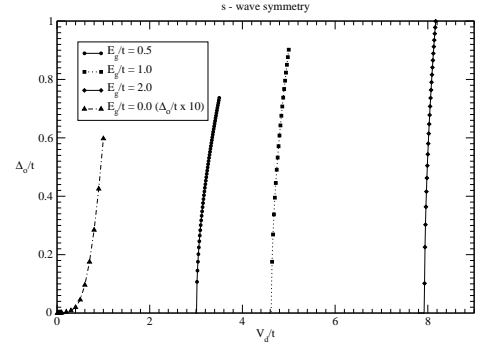


Figure 2. Δ_o/t vs V_d/t for several values of the pseudogap parameter, E_g/t . The superconducting order parameter, when $E_g = 0/t$ has been re-scaled by a factor of 10. For $E_g/t \neq 0$ there is a critical interaction potential, $V_d/t = V_{d,c}^{\Delta_o}/t$, below which $\Delta_o/t = 0$. For example, for $E_g/t = 0.50$ we find $V_{d,c}^{\Delta_o}/t \approx 3.00$ in units of t .

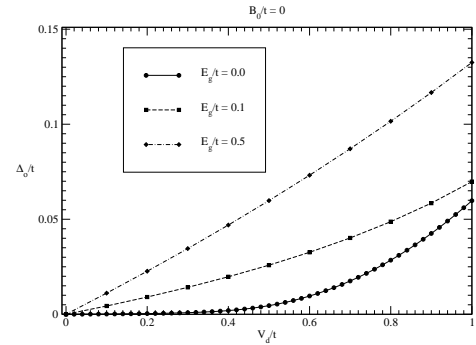


Figure 3. Δ_o vs V_d for several values of the pseudogap parameter, E_g . Following the approximation of Ref. [7], we have taken $B_o \equiv 0$

From Fig. 3 we plot Δ_o/t vs V_d/t for several values of the pseudogap parameter, E_g/t , when we adopt the approximation of Ref. [7], namely, $B_o/t \equiv 0$. This approximation does not produce a critical value of the interaction potential. In consequence, $V_d^{\Delta_o}/t = 0, \forall E_g/t$. As our Eq. (11) does not have the presence of the factor B_o/t , we cannot perform this approximation. Because of this, T_c/t always needs a critical value of the interaction, for $\forall E_g/t \neq 0$.

4 Discussion and conclusions

In this paper we have considered that the pseudogap and the superconducting order parameter both have the same sym-

metry, namely, pure s -wave symmetry. This is not a crazy idea, because it has been shown that the observed symmetry of the order parameter cannot be fitted with only the lowest harmonics of the d -wave order parameter [18, 19, 20, 21]. Furthermore, a recent experiment with twisted Josephson junctions in the Bi -cuprates [22], is in favor of an extended s -wave order parameter, and has shown the absence of a d -wave part in the order parameter. However, the inclusion of order parameters with another symmetry is not a difficult task in our working scheme. With this point of view in mind and following the model of Țifrea, Grosu and Crisan [7] we have studied their model to treat delicate points like the critical interaction potential.

In summary, we have numerically implemented a model which has a pseudogap (really, it is a semiconductor gap, since damping effects have been neglected in our calculations) in the one-particle energy spectrum of quasi-particles in the temperature range $0 \leq T \leq T^*$. We have investigated the effect of E_g on the two basic parameters of the BCS theory, T_c and Δ_o . We have found that for $E_g \neq 0$ two critical pairing potentials emerge from our calculations. In consequence, in order to define the ratio $R \equiv 2\Delta_o(V_d, E_g)/k_B T_c(V_d, E_g)$ we need to be above the bigger of the two critical pairing potentials. When $E_g = 0$, $R \approx 3.5$ in the BCS -approximation. We have briefly discussed the case when both order parameters, E_g and Δ_o , have the same symmetry, namely, pure s -wave symmetry. However, the d -wave symmetry is not difficult to study and we leave for a future publication. Another aspect we could study is the crossover phase diagram from the BCS limit to the Bose-Einstein regime [23].

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References

- [1] J. G. Bednorz and K. A. Müller, *Z. Phys. B* **64**, 189-193 (1986).
- [2] Th. A. Maier, M. Jarrel, A. Macridin, and F.-C. Zhang, *cond-mat/0208419* (submitted to *Phys. Rev. Lett.*).
- [3] J. L. Tallon and J. W. Loram, *Physica C* **349**, 53 (2001).
- [4] R. M. Dipasupil, M. Oda, N. Momono and M. Ido, *J. Phys. Soc. Jpn.* **71**, 1535-1540 (2002).
- [5] V. M. Krasnov et al. *Phys. Rev. Lett.* **84**, 5860 (2000)
- [6] D. Rubio Temprano, V. Trounov and K. A. Müller, *Phys. Rev. B* **66**, 184506 (2002). See also, P. Häfliger, A. Podlesnyak, K. Conder and A. Furrer, *PSI-Zürich Internal Report* (2003).
- [7] I. Țifrea, I. Grosu and M. Crisan, *Physica C* **371**, 104 (2002).
- [8] F. Pistolesi and Ph. Nozières, *Phys. Rev. B* **66**, 054501 (2002).
- [9] N. Andrenacci and H. Beck, *cond-mat/0304084*; *ibidem*, *Physica C* (to be published, Proceedings of the M2S-HTSC-VII).
- [10] M. H. Pedersen, J. J. Rodríguez-Núñez, H. Beck, T. Schneider and S. Schafroth, *Z. Phys. B* **103**, 21-28 (1997).
- [11] S. Schafroth and J. J. Rodríguez-Núñez, *Z. Phys. B* **102**, 493-499 (1997).
- [12] S. Schafroth, J. J. Rodríguez-Núñez and H. Beck, *J. Phys.: Condens. Matter* **9**, L111-L118 (1997).
- [13] Y.-J. Kao, A. P. Iyengar, Q. Chen and K. Levin, *Phys. Rev. B* 140505(R) (2001).
- [14] I. Kosztin, Q. Chen, B. Jankó and K. Levin, *cond-mat/9805065*.
- [15] K. Levin, Q. Chen, I. Kosztin, B. Jankó and A. Iyengar, *cond-mat/0107275*.
- [16] Y.-J. Kao, A. P. Iyengar, J. Stajic, and K. Levin, *cond-mat/0207004 v2*.
- [17] J. J. Rodríguez-Núñez, L. Sánchez, D. Romero and H. Beck (submitted).
- [18] V. M. Loktev, R. M. Quick and S. G. Sharapov, *Physics Reports* **349**, 1-123 (2001).
- [19] J. Mesot, M. R. Norman, H. Ding et al., *Phys. Rev. Lett.* **83**, 840-843 (1999), *ibidem.*, *cond-mat/9812377*.
- [20] R. Gat, S. Christensen, B. Frazer et al., *cond-mat/9906070*.
- [21] G. G. N. Angilella, A. Sudbo, and R. Pucci, *Eur. Phys. J. B* **15**, 269 (2000).
- [22] R. A. Klemm, G. Arnold, A. Bille et al, *Int. Mod. Phys. B* **13**, 3449-3454 (1999).
- [23] M. B. Soares, F. Kokubun, J. J. Rodríguez-Núñez and O. Rondón, *Phys. Rev. B* **65**, 174506 (2002); see also, A. Perali, P. Pieri, and G. C. Strinati, *Phys. Rev. B* **68**, 066501 (2003); J. Quintanilla and B. L. Györfy, *J. Phys. A: Math. Gen.* **36**, 9375 (2003).
- [24] J. J. Rodríguez-Núñez, O. Alvarez, E. Orozco, O. Rondón, F. Kokubun and M. B. Soares *Phys. Rev. B* **68**, 066502 (2003); O. Alvarez-Llamoza, E. Orozco and J. J. Rodríguez-Núñez (submitted).